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QUANTUM CHEMICAL CALCULATIONS OF Si-F-SPECIES

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The examination of the thermal decomposition of alkalihexafluorosilicates resulted in first conceptions about the diffusion of Si-F-species in the solid [1]. Starting from this reaction description semiempirical quantumchemical computation methods (CNDO/2, EHT) have been used to get informations about the stability and reactivity of SiF_4-, SiF_3^+ - and SiF_2^{2+} (SiF_2 resp.) - units.

The quantumchemical calculations show thal the existence of planar SiF_4 as well as planar SiF_3^+ in the solid can not be excluded from the energetical point of view. The additional stabilization of planar structures in the crystal should be responsible for this fact. A comparison between the calculated Si-F-species shows, that the bond energy of one Si-F-bond decreases with growing number of ligands and in this connection with decreasing F-Si-F-bond angle.The equilibrium distances of the Si-F-bonds found out with CNDO/2 - calculations decrease with increasing bond angle.

1 L. Kolditz, F. Janiak, W. Wilde, S. Sciesielski, S.Feist, Z.anorg.allg.Chem. 452 (1979) 43.